# Inverse problem in anomalous diffusion with uncertainty propagation

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Recently, Bevilacqua, Galeão and co-workers have developed a new analytical formulation for the simulation of diffusion with retention phenomena. This new formulation aims at the reduction of all diffusion processes with retention to a unifying model that can adequately simulate the retention effect. This model may have relevant applications in a number of different areas such as population spreading with partial hold up of the population to guarantee territorial domain chemical reactions inducing adsorption processes and multiphase flow through porous media. In this new formulation a discrete approach is firstly formulated taking into account a control parameter which represents the fraction of particles that are able to diffuse. The resulting governing equation for the modelling of diffusion with retention in a continuum medium requires a fourth-order differential term. Specific experimental techniques, together with an appropriate inverse analysis, need to be determined to characterize complementary parameters. The present work investigates an inverse problem which does not allow for simultaneous estimation of all model parameter. In addition a two-step characterization procedure proposed: in the first step the diffusion coefficient is estimated and in the second one the complementary parameters are estimated. In this paper, it is assumed that the first step is already completed and the diffusion coefficient is known with a certain degree of reliability. Therefore, this work is aimed at investigating the confidence intervals of the complementary parameters estimates considering both the uncertainties due to measurement errors in the experimental data and due to the uncertainty propagation of the estimated value of the diffusion coefficient. The inverse problem solution is carried out through the maximum likelihood approach, with the minimization problem solved with the Levenberg-Marquardt method, and the estimation of the confidence intervals is carried out through the Monte Carlo analysis.

Keywords: diffusion, inverse problems, uncertainty propagation, Monte Carlo method.

## **1. INTRODUCTION**

Spreading of particles or microorganisms immersed in a given medium or deployed on a given substratum is frequently modeled as a diffusion process, given by the well-known diffusion equation derived from Fick's second law. This model represents quite satisfactorily the behavior of several physical phenomena related to dispersion processes, but for some cases this approach fails to represent the real physical behavior. For instance, population spreading or dispersing particles may be partially and temporarily blocked when immersed in some particular media, an invading species may hold a fraction of the total population stationary on the conquered territory in order to guarantee territorial domain and chemical reactions may induce absorption processes for the solutes diffusion in liquid solvents in the presence of absorbent material [4]. Among other physicochemical phenomena that are in need of the analytical formulation improvement due to side effects not accounted for in the classical diffusion theory, we may cite the flows through porous media [11], and diffusion processes for some dispersing substances immersed in particular supporting media [1, 5, 6, 8, 14]. In most cases appearing in the literature addressing this issue, the well-known second-order parabolic equation is assumed as the basic governing equation of the dispersion process, but the anomalous diffusion effect is modeled with an introduction of fractional derivatives [13], or imposing an arbitrary variation of the diffusion coefficient with time or concentration [10, 18]. Nevertheless, in order to overcome the anomalous diffusion issue by imposing an artificial dependence of the diffusion coefficient on the particle concentration or introducing extra differential terms while keeping the second-order rank of the governing equation disguises the real physical phenomenon occurring in the process. In 2011, Bevilacqua, Galeão and co-workers derived a new analytical formulation for the simulation of anomalous diffusion phenomena [2], explicitly taking into account the retention effect in the dispersion process, aiming at the reduction of all diffusion processes with retention to a unifying phenomenon. The new parameters introduced, besides the diffusion coefficient, characterize the blocking process, and specific experimental techniques, together with an inverse analysis, need to be settled to determine these complementary parameters. The present work investigates an anomalous diffusion inverse problem which does not allow for simultaneous estimation of all model parameters [15]. In addition a two-step characterization procedure is proposed. It is considered possible to impose a case in which the blocking process does not take place, for instance as it occurs in the flow of ferrofluid in micro-channels [7]. In this example, the problem may or may not present an anomalous diffusion effect, depending on the presence of a magnetic field. Therefore, in the first step, assuming that all particles are able to diffuse, the diffusion coefficient of the model may be estimated. Then, the second step may be carried out in a situation in which anomalous diffusion occurs for the given problem, with the diffusion coefficient already characterized, in order to estimate the complementary anomalous diffusion parameters. In this paper, it is assumed that the first step of the two-step procedure is already completed and the diffusion coefficient is known with a certain degree of reliability. Therefore, this work is aimed at investigating the confidence intervals of the complementary parameters estimates, considering the uncertainties due to measurement errors in the experimental data and due to the uncertainty propagation of the considered value of the diffusion coefficient. The inverse problem solution is carried out through the maximum likelihood approach, with the minimization problem solved with the Levenberg-Marquardt method [12], and the estimation of the confidence intervals is carried out through the Monte Carlo analysis [9].

# 2. PROBLEM FORMULATION AND SOLUTION METHODOLOGY

Let us consider the process schematically represented in Fig. 1. The redistribution of the contents of each cell indicates that the fraction of the contents  $\alpha p_n$  is retained in the  $n^{th}$  cell and the exceeding volume is evenly transferred to the neighboring cells, that is,  $0.5\beta p_n$ , to the  $(n-1)^{th}$  cell on the left and to the  $(n+1)^{th}$  cell on the right, at each time step, where  $\beta = 1 - \alpha$ . This means that the dispersion runs slower than for the classical diffusion problem. Note that if  $\beta = 1$ , the problem is reduced to the classical Gaussian distribution.

This process can be written as the following algebraic expressions:

$$p_n^t = (1 - \beta)p_n^{t-1} + \frac{1}{2}\beta p_{n-1}^{t-1} + \frac{1}{2}\beta p_{n+1}^{t-1}, \tag{1}_1$$

$$p_n^{t+1} = (1-\beta)p_n^t + \frac{1}{2}\beta p_{n-1}^t + \frac{1}{2}\beta p_{n+1}^t.$$
(1)<sub>2</sub>



Fig. 1. Schematic representation of the symmetric distribution with retention  $\alpha = (\beta - 1)$ .

Manipulating Eqs.  $(1)_1$  and  $(1)_2$  in order to obtain finite difference terms yields:

$$\frac{\Delta p_n^{t+\Delta t}}{\Delta t} = \beta \left\{ \frac{1}{2} \frac{L_0^2}{T_0} \frac{\Delta^2 p_n}{\Delta x^2} + \frac{O\left(\Delta x^2\right)}{\Delta x^2} - (1-\beta) \frac{1}{4} \frac{L_1^4}{T_0} \frac{\Delta^4 p_n}{\Delta x^4} \right\}^{t-\Delta t},\tag{2}$$

where  $T_0$ ,  $L_0$  and  $L_1$  are integration parameters. Calling  $K_2 = L_0^2/2T_0$  and  $K_4 = L_1^4/4T_0$ , both considered constant in this work, and using the limit as  $\Delta x \to 0$  and  $\Delta t \to 0$ , we have:

$$\frac{\partial p(x,t)}{\partial t} = \beta K_2 \frac{\partial^2 p(x,t)}{\partial x^2} - \beta (1-\beta) K_4 \frac{\partial^4 p(x,t)}{\partial x^4}.$$
(3)<sub>1</sub>

The fourth-order differential term with a negative sign introduces the anomalous diffusion effect, which appears naturally without any artificial assumption, as an immediate consequence of the temporary retention imposed by the redistribution law. Further discussion on the model derivation can be found in [2].

As a test case for the present work, we consider the governing equation given in Eq. (3)<sub>1</sub> valid for 0 < x < 1 and t > 0, with the following boundary and initial conditions:

$$p(0,t) = 1, \qquad p(1,t) = 1, \qquad \left. \frac{\partial p(x,t)}{\partial x} \right|_{x=0} = 0, \qquad \left. \frac{\partial p(x,t)}{\partial x} \right|_{x=1} = 0, \qquad t > 0, \tag{3}_2$$

$$p(x,0) = f(x) = 2\sin^{100}(\pi x) + 1, \qquad 0 \le x \le 1.$$
 (3)<sub>3</sub>

The problem given in Eqs. (3) is solved in this work with NDSolve routine of the Mathematica platform, under automatic absolute and relative error control. When it comes to inverse problem solution by observing the problem defined in Eqs. (3), it is evident that the three parameters appearing in the model cannot be estimated simultaneously since in Eq. (3)<sub>1</sub> there are three parameters defining two coefficients, i.e., there are infinite sets of values for the parameters  $\mathbf{Z} = \{\beta, K_2, K_4\}$ that lead exactly to the same mathematical formulation, yielding non-uniqueness of the inverse problem solution, which was also illustrated by means of a sensitivity analysis in [15]. Since the most interesting aspect of the previously described problem would be the identification of the three parameters appearing in the model, due to their direct physical interpretation [2], we choose not to rewrite the problem in terms of only two coefficients which would multiply the second- and fourthorder differential terms. Next, we shall consider that the parameter  $K_2$  can be obtained through an independent experiment, for example, by means of an inverse problem in a physical situation where the blocking process that characterizes the anomalous diffusion phenomenon does not occur, i.e.,  $\beta = 1$ . Then, the main goal becomes to estimate  $\beta$  and  $K_4$ , and to provide an accurate uncertainty analysis due to errors in the experimental data and in the considered value of  $K_2$ . The inverse problem formulation and solution are addressed in the following sections.

## 3. INVERSE PROBLEM FORMULATION AND SOLUTION

In order to investigate the inverse problem solution concerning the estimation of the three model parameters,  $\mathbf{Z} = \{\beta, K_2, K_4\}$ , we consider a vector of experimental data  $\mathbf{Y}$ , simulated with the solution of Eq. (3), and the addition of noise simulated from a normal distribution with known variance:

$$Y_i = p_i(\mathbf{Z}_{exact}) + \epsilon_i, \qquad \epsilon \sim N(0, \sigma_e^2). \tag{4}$$

In this case, the maximum likelihood approach leads to the ordinary least squares norm as objective function, given by the sum of the squared residues between the experimental data  $Y_i$  and the predicted values from the solution of Eq. (3),  $p_i(\mathbf{Z})$ :

$$S(\mathbf{Z}) = \sum_{i=1}^{N_d} (p_i(\mathbf{Z}) - Y_i)^2.$$
 (5)

So, the vector  $\mathbf{Z}$  that minimizes S yields the maximum likelihood estimates for the model parameters under investigation. In order to minimize the previously presented objective function, we use in this work the Levenberg-Marquardt method [12]. Starting with an initial guess  $\mathbf{Z}_0$ , an iterative procedure is constructed, in which new estimates are obtained with

$$\mathbf{Z}_{n+1} = \mathbf{Z}_n + \Delta \mathbf{Z}_n, \qquad n = 0, 1, 2, \dots, \tag{6}$$

being the correction  $\Delta \mathbf{Z}_n$  calculated from

$$\Delta \mathbf{Z}_n = -\left[\mathbf{J}_n^T \mathbf{J}_n + \lambda_n \mathbf{I}\right]^{-1} \mathbf{J}_n^T \mathbf{R}_n,\tag{7}$$

where  $\lambda$  is a damping parameter, **I** is the identity matrix and the elements of the sensitivity matrix **J**, known as the sensitivity coefficients, are

$$J_{ij} = \frac{\partial p_i}{\partial Z_j}, \qquad i = 1, 2, ..., N_d, \qquad j = 1, 2, ..., N_p,$$
(8)

where  $N_p$  is the number of parameters being estimated, i.e., the dimension of the vector  $\mathbf{Z}$  and  $\mathbf{R}$  is the vector of residues, whose elements are given by

$$R_i = p_i(\mathbf{Z}) - Y_i, \qquad i = 1, 2, ..., N_d.$$
(9)

The iterative procedure of sequentially calculating  $\Delta \mathbf{Z}_n$  and  $\mathbf{Z}_{n+1}$  with Eqs. (7) and (6), respectively, is continued until the convergence criterion

$$\Delta \mathbf{Z}_{n,j} | < \epsilon_{tol}, \qquad \text{for} \qquad j = 1, 2, \dots, N_p \tag{10}$$

is satisfied, where  $\epsilon_{tol}$  is a prescribed tolerance. The damping factor  $\lambda_n$  is varied during the iterative procedure, such that when convergence is achieved its value is close to zero.

The derivatives that must be calculated in order to obtain the sensitivity coefficients in Eq. (8) can be computed with a finite difference scheme. Nevertheless, the finite difference approximations must be employed with care because of the choice of the increment. If a large value is used, it is possible that the approximations will not be sufficiently accurate. On the other hand, if very small values are used for the increment, large numerical errors can occur due to the difference of numbers very close to each other, motivating the use of more involved techniques for the computation of the sensitivity coefficients, such as the complex-step method [17] or the derivation and solution of the sensitivity coefficient equations [3]. The sensitivity equations have been derived in [15], yielding for  $X_{\beta}$ 

$$\frac{\partial X_{\beta}(x,t)}{\partial t} - \beta K_2 \frac{\partial^2 X_{\beta}(x,t)}{\partial x^2} + \beta (1-\beta) K_4 \frac{\partial^4 X_{\beta}(x,t)}{\partial x^4} = K_2 \frac{\partial^2 p(x,t)}{\partial x^2} - (1-\beta) K_4 \frac{\partial^4 p(x,t)}{\partial x^4} + \beta K_4 \frac{\partial^4 p(x,t)}{\partial x^4}, \qquad (11)_1$$

$$X_{\beta}(0,t) = 0, \qquad X_{\beta}(1,t) = 0, \qquad \left. \frac{\partial X_{\beta}(x,t)}{\partial x} \right|_{x=0} = 0, \qquad \left. \frac{\partial X_{\beta}(x,t)}{\partial x} \right|_{x=1} = 0, \tag{11}_2$$

$$X_{\beta}(x,0) = 0,$$
 (11)<sub>3</sub>

for  $X_{K_2}$ ,

$$\frac{\partial X_{K_2}(x,t)}{\partial t} - \beta K_2 \frac{\partial^2 X_{K_2}(x,t)}{\partial x^2} + \beta (1-\beta) K_4 \frac{\partial^4 X_{K_2}(x,t)}{\partial x^4} = \beta \frac{\partial^2 p(x,t)}{\partial x^2}, \tag{12}$$

$$X_{K_2}(0,t) = 0, \qquad X_{K_2}(1,t) = 0, \qquad \frac{\partial X_{K_2}(x,t)}{\partial x}\Big|_{x=0} = 0, \qquad \frac{\partial X_{K_2}(x,t)}{\partial x}\Big|_{x=1} = 0, \qquad (12)_2$$

$$X_{K_2}(x,0) = 0 (12)_3$$

and for  $X_{K_4}$ 

$$\frac{\partial X_{K_4}(x,t)}{\partial t} - \beta K_2 \frac{\partial^2 X_{K_4}(x,t)}{\partial x^2} + \beta (1-\beta) K_4 \frac{\partial^4 X_{K_4}(x,t)}{\partial x^4} = -\beta (1-\beta) \frac{\partial^4 p(x,t)}{\partial x^4}, \tag{13}$$

$$X_{K_4}(0,t) = 0, \qquad X_{K_4}(1,t) = 0, \qquad \frac{\partial X_{K_4}(x,t)}{\partial x}\Big|_{x=0} = 0, \qquad \frac{\partial X_{K_4}(x,t)}{\partial x}\Big|_{x=1} = 0, \qquad (13)_2$$

$$X_{K_4}(x,0) = 0. (13)_3$$

 $X_{Z_j}(x,t) = \partial p(x,t)/\partial Z_j$ . Equations (11)–(13) can be numerically solved for the sensitivity coefficients  $X_{\beta}(x,t)$ ,  $X_{K_2}(x,t)$  and  $X_{K_4}(x,t)$ , respectively, after the computation of p(x,t), with the same methodology that was employed in the solution of the direct problem, i.e., using *NDSolve* routine of the *Mathematica* platform, under automatic absolute and relative error control. After this, the coefficients of the matrix **J**, Eq. (8), can be readily computed.

It should also be highlighted that the sensitivity analysis plays a major role in several aspects related to formulation and solution of inverse problems [3]. In order to obtain good estimates, within reasonable confidence intervals, it is required for the sensitivity coefficients to be relatively high and, when two or more unknowns are simultaneously estimated, their sensitivity coefficients must be linearly independent, what graphically means that they should not present the same slope in absolute value. Otherwise  $|\mathbf{J}^T \mathbf{J}| \approx 0$  and the problem is ill-conditioned. Since the problem investigated in this work involves parameters with different orders of magnitude, the scaled sensitivity coefficients are employed in order to allow for more evident comparisons between the sensitivity coefficients with respect to different parameters and identification of linear dependence. The scaled sensitivity coefficients are obtained by multiplying the sensitivity coefficient by an estimate or reference value for the value of the concerned parameter, i.e.  $\overline{X}_{Z_i} = Z_i \frac{\partial p}{\partial Z_i}$ . Therefore, we have:

$$\overline{X}_{\beta}(x,t) = \beta \frac{\partial p(x,t)}{\partial \beta}, \qquad \overline{X}_{K_2}(x,t) = K_2 \frac{\partial p(x,t)}{\partial K_2}, \qquad \overline{X}_{K_4}(x,t) = K_4 \frac{\partial p(x,t)}{\partial K_4}.$$
(14)

In this work, it is assumed that the parameter  $K_2$  has already been estimated through an independent previous procedure, for instance when conducting an experiment in which the blocking process is known not to occur. Therefore, assuming prior information on the parameter  $K_2$  is available (mean and confidence interval), the goal is to obtain estimates for the parameters  $\beta$  and  $K_4$ and assess their joint confidence region as a result of uncertainty in the assumed value of  $K_2$  and measurement errors. In order to calculate the confidence intervals for the parameters  $\beta$  and  $K_4$ , the inverse problem of estimating  $\beta$  and  $K_4$  is solved through the minimization of the maximum likelihood objective function, Eq. (5), assuming that the parameter  $K_2$  is known. In order to calculate the confidence of the estimated parameters, and taking into account the uncertainty in the given value of  $K_2$ , the Monte Carlo error propagation analysis is introduced [9]. The idea is to simulate M virtual noisy experiments, employing different values of  $K_2$  (randomly simulated from the a priori known probability distribution), and different simulated experimental data, and then examine the statistics of the corresponding estimated parameters. This procedure can be seen while solving the inverse problem several times, and for every time it is solved all inputs (experimental data and  $K_2$  in this case) are varied randomly within their uncertainty limits, obeying their known statistical distributions, independent of the others. After a sufficiently large number of independent calculations are performed, the distribution of the computed results (the estimated values of  $\beta$  and  $K_4$  in this case) nearly describes the distribution of all possible results from the combination of the input data.

#### 4. Results and discussion

In the following consider the case with  $\beta = 0.2$ ,  $K_2 = 10^{-3}$  and  $K_4 = 10^{-5}$  in Eq. (3)<sub>1</sub>. This test case is investigated in [15] and it is shown that for t > 95 the sensitivity coefficients become essentially constant, suggesting that measurements beyond that time may not aggregate useful information for the inverse problem solution. The influence of the measurement location on sensitivity coefficients is also investigated in the present work. For instance, consider Fig. 2, which depicts the scaled sensitivity coefficients with respect to the three parameters,  $\beta$ ,  $K_2$ , and  $K_4$ , at t = 10, for  $0 \le x \le 1$ .



Fig. 2. Sensitivity coefficients along the spatial domain x at t = 10.

It can observed in this figure that  $x_m = 0.5$  may be the best position for performing transient measurements concerning the inverse problem solution. In the present work, besides  $x_m = 0.5$ , the use of transient measurements acquired with a single sensor at  $x_m = 0.4$  and  $x_m = 0.45$  is also investigated, for the inverse problem solution, in order to illustrate the influence of the measurement position choice on the confidence intervals of the estimates. In all the results presented hereafter 90 experimental data for the inverse problem solution are considered, obtained from t = 5 up to t = 95, using a single sensor located at: (i) case 1:  $x_m = 0.5$ , (ii) case 2:  $x_m = 0.4$ , and (iii) case 3:  $x_m = 0.45$ . For instance, Fig. 3 illustrates a set of experimental data at  $x_m = 0.5$ , simulated by employing Eq. (4) with  $\sigma_e = 0.02$ , yielding, on average, up to 4% of noise in the data. In this figure, together with the experimental data, the curve obtained from the solution of problem (3) for the test case under consideration is also plotted.



Fig. 3. Simulated experimental data (red dots) for transient measurements of a sensor located at x = 0.5. The black curve shows the numerical solution employed to simulate the experimental data.

In the present work, for each of the three measurement positions considered ( $x_m = 0.5$ ,  $x_m = 0.4$ , and  $x_m = 0.45$ , named case 1, 2 and 3, respectively), M = 500 virtual noisy experiments have been simulated employing  $\sigma_e = 0.02$  in Eq. (4), and for each simulated independent experiment, different values of  $K_2$  have been employed, randomly obtained from a normal distribution with  $10^{-3}$  mean and  $0.1 \times 10^{-3}$  standard deviation (10% of the mean value), which means the 95% confidence interval for  $K_2$  is  $[0.8 \times 10^{-3}, 1.2 \times 10^{-3}]$ . This information concerning  $K_2$  is supposed to be obtained in the first step of the procedure herein proposed, in an experiment where the blocking process does not occur and the diffusion coefficient can be estimated. The goal here is to investigate how this uncertainty of the value of  $K_2$  propagates into the estimates of  $\beta$  and  $K_4$ , in the presence of measurement errors, in the second step, now considering an experiment with anomalous diffusion and with this a priori information available for the parameter  $K_2$ .

First, Fig. 4a illustrates the histogram plotted from 500 values of  $K_2$  employed in the simulations for case 1. For a sufficiently large number of simulations, this histogram approaches the exact normal distribution from which the values of  $K_2$  have been sampled. In fact, Fig. 4a demonstrates that with 500 experiments a fairly good approximation of the distribution considered to be known for this distribution is obtained. In fact, the 95% confidence interval calculated from these 500 samples illustrated in Fig. 4a is  $[0.804 \times 10^{-3}, 1.196 \times 10^{-3}]$ , which is very close the exact interval which is  $[0.8 \times 10^{-3}, 1.2 \times 10^{-3}]$ . Figures 4b and 4c depict the corresponding histograms for the estimates of the parameters  $\beta$  and  $K_4$ , respectively, obtained from 500 simulated noisy experiments. It should be noted that both histograms for  $\beta$  and  $K_4$  seem to be slightly asymmetric with respect to the mean. Whilst this can be a collateral effect of the approximation obtained with a limited number of simulated experiments, it can be also due to the nonlinearity of the problem, which means that even if both the experimental errors and the assumed values of  $K_2$  are normally distributed, the statistical distributions of the estimated parameters  $\beta$  and  $K_4$  are not necessarily normal.



Fig. 4. Histogram of: a) sampled values of  $K_2$ , b) estimates of  $\beta$ , c) estimates of  $K_4$ .

Looking at the investigation of the influence of the measurement position on the reliability of the estimates, we see that Fig. 5 shows the elliptic joint confidence intervals for the estimated parameters  $\beta$  and  $K_4$  for the three cases studied in this work: case 1:  $x_m = 0.5$ , case 2:  $x_m = 0.4$ , and case 3:  $x_m = 0.45$ . A direct comparison of these three confidence regions shows that the measurements performed at  $x_m = 0.5$  produce the most reliable estimates, whereas the measurements performed at  $x_m = 0.4$  produce the least reliable estimates. It is interesting to notice that this effect is much more evident in the estimation of  $K_4$ . It should be noted that the elliptic confidence region becomes narrow much more in the vertical direction of the graph  $(K_4)$  than in the horizontal direction of the graph  $(\beta)$ .



Fig. 5. Direct comparison of the elliptic joint confidence regions for  $\beta$  and  $K_4$  estimated in cases 1, 2 and 3.

The influence of the measurement position on the reliability of the estimates is better quantified in Table 1, which besides the mean estimates and confidence intervals for each case, also shows the ratio between the standard deviation and the mean for each distribution. Recalling that this ratio was 10% in the assumed estimation of  $K_2$ , it can be concluded that the uncertainties were not greatly amplified into the estimates for  $\beta$  and  $K_4$ , noting that for case 1 their calculated ratios are 11.38% and 11.89%, which besides the uncertainty of  $K_2$  also include the effect of the measurement errors. Nonetheless, if another, less favorable measurement position is chosen (cases 2 or 3, for instance), these ratios increase remarkably, especially for  $K_4$ . This clearly illustrates the importance of the adequate choice of the experimental measurements employed for the inverse problem solution.

Meas. position	β	$\frac{\sigma_{\beta}}{\mu_{\beta}} \times 100\%$	$K_4 \times 10^5$	$\frac{\sigma_{K_4}}{\mu_{K_4}} \times 100\%$
Case 1, $x_m = 0.5$	0.203[0.154, 0.246]	11.38%	0.994[0.764, 1.24]	11.89%
Case 2, $x_m = 0.4$	0.201[0.150, 0.250]	12.39%	1.01[0.652, 1.35]	17.14%
Case 3, $x_m = 0.45$	0.202[0.152, 0.248]	12.00%	1.00[0.678, 1.32]	16.00%

**Table 1.** Estimated mean and 95% confidence intervals for  $\beta$  and  $K_4$ .

## 5. CONCLUSIONS

The inverse problem formulation and solution for two unknowns,  $K_4$  and  $\beta$ , were investigated in relation to a new analytical formulation for the simulation of the phenomena of anomalous diffusion. The investigated inverse problem does not allow for the simultaneous estimation of all three parameters and a characterization procedure in two steps is proposed. The reliability of the anomalous diffusion parameters estimates is studied concerning the uncertainty in the experimental data as well as the propagation of error concerning the value of the diffusion coefficient, estimated in the first step. The inverse analysis was carried out for transient measured experimental data obtained with a single sensor, whose position was investigated with respect to the corresponding estimates obtained. The results show that the errors present in the inputs do not amplify significantly into the estimates of the anomalous diffusion parameters. Nevertheless, location and time interval in which the measured data are acquired in order to be employed in the inverse problem solution have to be chosen with care, since they affect remarkably the reliability of the estimates.

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